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Author(s): Velizhanin, Kirill A.

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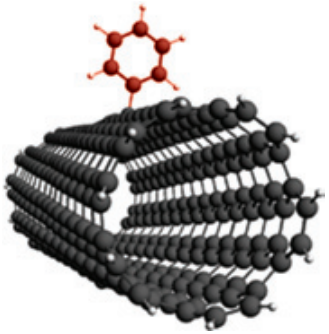
Final 2016 IC report for w15_cnanostruct

"Optical and Transport Properties of Carbon-Based Nanostructures: A Density Functional Theory Study"

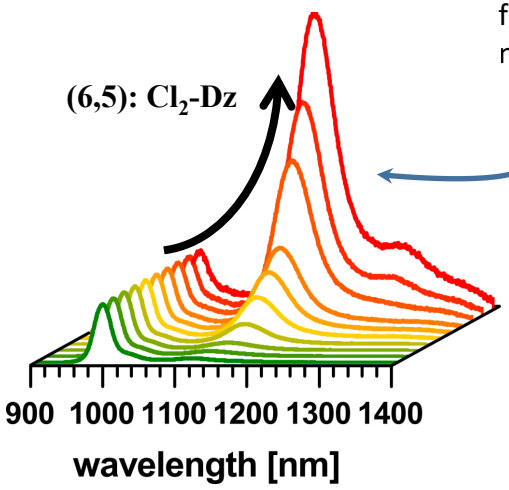
PI: Kirill A. Velizhanin

- Functionalized carbon nanotubes



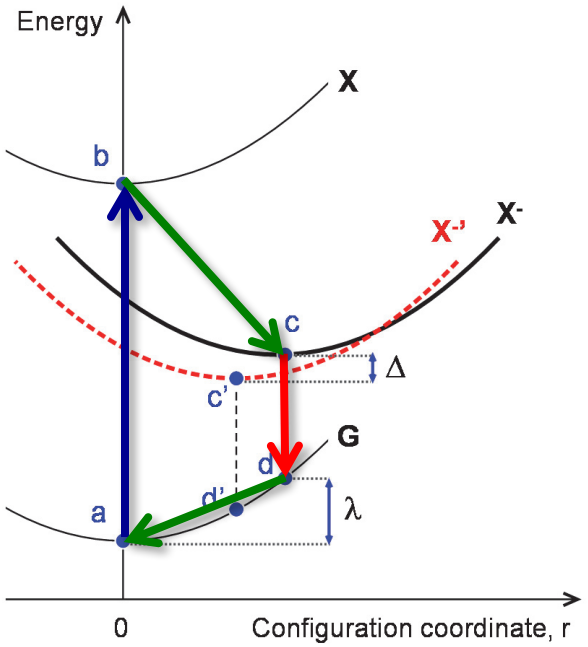
Covalent functionalization of carbon nanotubes holds promise for enhancing electronic and optical properties – relevant for electronics, optoelectronics and light-emitting applications.

For example, increasing covalent functionalization can drastically ncrease the photoluminescence quantum yield



Density functional theory computations, supported by IC Computing, allowed us to come up with this diagram for the electronic structure of functionalized SWCNT, which accurately reproduce experimental observations

- "Molecular" level diagram



Blue – E_{11} absorption/emission
Red – E_{11}^{-} emission
Green – intraband relaxation